

can say that the insertion of these synthetic additives lower the temperature of the structural phase transitions comparative to pure lipids and in many cases induce the formation of cubic phases at low temperatures, e.g. 30°C, which corresponds to an increase of the lipid matrix surface curvature. The scattering patterns of the cubic phases are clearly identifiable, despite their intrinsic low resolution. In some cases micellar cubic phases were observed.

In this study we shifted our attention to the influence of small molecules such as urea and TMAO. It is accepted that they have antagonistic effects on the fluidity of lipid membranes. In red blood cells, urea slightly increases the gel-phase domains, but this effect is counteracted by TMAO. We intended to determine how these organic solutes affect the structure of a lipid membrane and determine their contribution to the possible curvature induced on them. We could see a change on the temperature of phase transitions and the formation of induced phases or structures.

#### 429-Pos Board B209

##### DPPC Monolayers Exhibit an Additional Phase Transition at High Surface Pressure

**Chen Shen**<sup>1</sup>, Jorge B. de la Serna<sup>2,3</sup>, Bernd Struth<sup>4</sup>, Beate Klösgen<sup>1</sup>.

<sup>1</sup>Dept. Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense, Denmark, <sup>2</sup>FKF&BMB, University of Southern Denmark, Odense, Denmark, <sup>3</sup>Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, United Kingdom, <sup>4</sup>Deutsches Elektronen-Synchrotron, Hamburg, Germany.

Pulmonary surfactant forms a monolayer at the air/aqueous interface within the lung. During the breath process, the surface pressure ( $\Pi$ ) periodically varies from ~40mN/m up to ~70mN/m. The film is mechanically stable during this rapid and reversible expansion.

Pulmonary surfactant consists of ~90% of lipid with 10% integrated proteins. Among its lipid compounds, di-palmitoyl-phosphatidylcholine (DPPC) dominates (~45wt%). DPPC is the only known lipid that can be compressed to very high surface pressure (~70mN/m) before its monolayer collapses. Most probably, this feature contributes to the mechanical stability of the alveoli monolayer. Still, to the best of our knowledge, some details of the compression isotherm presented here and the related structures of the DPPC monolayer were not studied so far.

The liquid-expanded/liquid-condensed phase transition of the DPPC monolayer at ~10mN/m is well known. Here, we report a second phase transition at elevated surface pressure (~50mN/m). The lateral structure of the monolayer at selected states (8mN/m, 20mN/m, 30mN/m, 40mN/m, 50mN/m, 60mN/m, 70mN/m; covering the whole pressure range of the isotherm) was investigated by grazing incidence X-ray diffraction (GIXD). The results report on the 2D packing lattice and on the inter-chain distance  $d_{xy}$ . Moreover, the tilt angle of the palmitoyl chains was calculated combining the lattice parameters and the geometrical boundary conditions. The course of the inter-chain distance versus surface pressure exhibits two regimes, separated by the phase transition.

#### 430-Pos Board B210

##### High Resolution Structure of the Ripple Phase of DMPC Bilayers

Kiyotaka Akabori, John F. Nagle.

Physics, Carnegie Mellon University, Pittsburgh, PA, USA.

We have obtained the most detailed ripple phase structure of dimyristoylphosphatidylcholine (DMPC) bilayers by taking synchrotron low and wide angle X-ray scattering (LAXS and WAXS) from highly aligned multilamellar samples. Our LAXS data have 52 measured reflections from which a two-dimensional electron density map was obtained at higher resolution than earlier maps obtained from less than half as many reflections. Consistent with the previous lower resolution study, the bilayer has a ripple amplitude of 18.5 Å with a thicker and longer major arm and a thinner and shorter minor arm, but the features are sharper allowing better estimates for the modulated bilayer profile and the distribution of headgroups along the aqueous interface. WAXS scattering, employing both grazing incidence and transmission geometry, revealed two sharp Bragg rod reflections with small out-of plane  $q_z$  components, narrow in-plane  $q_x$  width consistent with high lateral order, and a breadth in  $q_y$  consistent with tight coupling of the chains from opposite monolayers. Analysis shows that the major arm hydrocarbon chains are tilted in the ripple plane by 18° with respect to the local bilayer normal, contrary to a previous experimental interpretation. Each chain is tilted toward a next nearest neighbor similarly to the gel  $L_{\beta F}$  phase rather than the more usual  $L_{\beta I}$  phase. There was no clear signature in the WAXS data relating to the minor arm, consistent with those chains being disordered. However, based on the head-group electron density, we propose that the minor arm is not just like the fluid  $L_{\alpha}$  phase, as often supposed in the literature, because the maximum chain disorder is offset laterally between the upper and lower monolayers. This

asynchronous monolayer modulated melting suggests a direction for better theories of the ripple phase.

#### 431-Pos Board B211

##### Cation Effects on Zwitterionic Lipid Multilayers

**Merrell A. Johnson**<sup>1</sup>, Soenke Seifert<sup>2</sup>, Horia I. Petrache<sup>1</sup>.

<sup>1</sup>Physics, IUPUI, Indianapolis, IN, USA, <sup>2</sup>X-ray Science Division, Argonne National Laboratory, Argonne, IL, USA.

Lipid multilayers are found inside eukaryotic cells, as for example in the structure of the Golgi apparatus and around neurons forming myelin sheets. In laboratory, lipid multilayers form even in the absence of proteins. This is due to attractive van der Waals (vdW) forces that are strong enough to balance repulsive forces. In the current model of interbilayer interactions there are three contributions to intermembrane repulsion: electrostatics, bilayer shape fluctuations, and hydration. In this study we use small-angle x-ray scattering, dynamic light scattering, and theory to describe how these forces change in the presence of monovalent ions solution, in particular in the case of lithium ions for which the effects are significantly different than for sodium and potassium.

#### 432-Pos Board B212

##### Atomically Detailed Lipid Bilayer Models for the Interpretation of Scattering Data

Joseph Fogarty, Jianjun Pan, Sagar A. Pandit.

Physics, University of South Florida, Tampa, FL, USA.

We present a new atom density profile model (ADP) for extracting lipid bilayer structural characteristics from scattering data. Bilayer models are optimized using a high dimensional non-linear optimization method to simultaneously fit small angle neutron (SANS) and X-ray (SAXS) scattering data. Final results are determined from a statistical analysis of many optimized models. This approach yields data which indicates the precision with which the model and target data set determine structural properties. The model and methods are generalizable to more complex systems, such as bilayers with mixed lipid composition, asymmetric leaflets, or embedded transmembrane proteins.

#### 433-Pos Board B213

##### Van Der Waals Interactions of Lipid Membranes in Highly Polarizable Solutions

**Ryan Z. Lybarger**, Horia I. Petrache.

Department of Physics, Indiana University Purdue University Indianapolis, Indianapolis, IN, USA.

The van der Waals attraction between lipid membranes depends on the polarizability of solute molecules present in the aqueous space between neighboring membranes [1]. It has been shown that zwitterionic molecules (such as common pH buffers) affect van der Waals forces more strongly than monovalent salt ions [2]. Experimentally, changes in van der Waals forces are detected by x-ray scattering measurements of multilamellar lipid vesicles through the sensitivity of lamellar repeat distances to solution polarizabilities. In this respect, a direct determination of solute polarizabilities would lend support to the interpretation of x-ray data. Previously, we used a method to quantify the polarizabilities of zwitterionic pH buffers by combining mass density and index of refraction to calculate a dimensionless solution function,  $r(c)$ , which gives the polarizability of hydrated solutes as a function of concentration ( $c$ ) [3]. Here we present a similar analysis of TAPS (a zwitterionic buffer) and adenosine triphosphate (ATP). [1] V. Adrian Parsegian. Van der Waals Forces: A handbook for Biologists Chemists, Engineers, and Physicists. Cambridge University Press, 2006. [2] Megan M. Koerner, Luis A. Palacio, Johnnie W. Wright, Kelly S. Schweitzer, Bruce D. Ray, and Horia I. Petrache. Electrostatics of lipid membrane interactions in the presence of zwitterionic buffers. *Biophys. J.*, 101:362-369, 2011. [3] Krzysztof Szymanski and Horia I. Petrache. Composite polarizability and the construction of an invariant function of refraction and mass density for solutions. *J. Chem. Phys.*, 134(144701):7, 2011.

#### 434-Pos Board B214

##### Chelating Agent Induction of Multiphase Coexistence in Lipid Multilayers

**Michael Weisman**, Merrell A. Johnson, Bruce D. Ray, Horia I. Petrache.

Physics, Indiana University Purdue University Indianapolis, Indianapolis, IN, USA.

Previous work on lipid interactions has shown that zwitterionic buffers affect the attractive and repulsive forces between bilayers. The equilibrium spacing between lipid multilayers as measured by small angle x-ray scattering is determined by the balance of van der Waals (vdW), electrostatic and fluctuation forces. We will present a series of small angle x-ray scattering experiments